LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020124\
Data File : BF137232.D
Acq On : 01 Feb 2024 15:22
Operator : CG\JU
Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MMW-001

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137232.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	11	15	26	rBV2	39417	72340	3.12%	0.574%
2	3.893	300	307	314	rVB2	24538	37162	1.60%	0.295%
3	4.463	401	404	411	rVB	25152	28688	1.24%	0.228%
4	5.422	563	567	575	rBV	824881	788010	33.95%	6.254%
5	5.575	590	593	597	rVB	74583	70303	3.03%	0.558%
6	6.416	733	736	747	rBV	477296	463279	19.96%	3.677%
7	6.792	796	800	806	rBV	402431	354770	15.28%	2.816%
8	6.851	806	810	812	rVV	102173	89134	3.84%	0.707%
9	7.192	859	868	874	rBV2	63540	119000	5.13%	0.944%
10	7.351	889	895	904	rBV	1234226	1291487	55.63%	10.250%
11	7.598	931	937	942	rBV	73966	119297	5.14%	0.947%
12	7.904	978	989	994	rBV5	31824	74090	3.19%	0.588%
13	7.951	994	997	1005	rVB7	14505	25696	1.11%	0.204%
14	8.069	1013	1017	1025	rVB	550586	461388	19.88%	3.662%
15	8.145	1025	1030	1033	rBV	42990	41436	1.78%	0.329%
16	8.216	1033	1042	1045	rBV2	82001	178102	7.67%	1.414%
17	8.428	1071	1078	1082	rBV2	107792	211290	9.10%	1.677%
18	8.486	1085	1088	1089	rVV3	64065	79669	3.43%	0.632%
19	8.534	1093	1096	1103	rVB4	119372	151804	6.54%	1.205%
20	8.592	1103	1106	1111	rVB4	43640	53647	2.31%	0.426%
21	8.639	1111	1114	1119	rVB	51592	44417	1.91%	0.353%
22	8.698	1121	1124	1127	rVB3	25488	24233	1.04%	0.192%
23	8.739	1127	1131	1135	rBV6	19612	29210	1.26%	0.232%
24	8.786	1135	1139	1142	rBV4	31310	42961	1.85%	0.341%
25	8.916	1159	1161	1165	rVB5	19103	26057	1.12%	0.207%
26	9.151	1196	1201	1204	rBV	2526555	2321393	100.00%	18.424%
27	9.245	1214	1217	1219	rBV	56158	45152	1.95%	0.358%
28	9.269	1219	1221	1224	rVV	36638	33382	1.44%	0.265%
29	9.328	1228	1231	1237	rVB	57030	59786	2.58%	0.475%
30	9.822	1311	1315	1323	rVB	640866	539506	23.24%	4.282%
31	10.122	1364	1366	1370	rVB	51269	42142	1.82%	0.334%
32	10.257	1386	1389	1396	rVB	270247	247471	10.66%	1.964%
33	10.328	1397	1401	1406	rVB2	32638	40761	1.76%	0.324%
34	10.616	1446	1450	1462	rBV	1533999	1355339	58.38%	10.757%
35	11.316	1565	1569	1574	rBV	540518	462697	19.93%	3.672%
36	11.857	1657	1661	1666	rBV2	90197	108296	4.67%	0.860%

LSC Area Percent Report

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Data File : BF137232.D
Acq On : 01 Feb 2024 15:22
Operator : CG\JU
Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.898	1666	1668	1674	rVB4	29528	38442	1.66%	0.305%
38	11.969	1677	1680	1684	rBV5	16440	25362	1.09%	0.201%
39	12.569	1777	1782	1790	rBV	61645	86499	3.73%	0.687%
40	12.645	1792	1795	1806	rVB3	33463	48374	2.08%	0.384%
41	12.916	1836	1841	1844	rBV	1658599	1497275	64.50%	11.883%
42	13.833	1993	1997	2003	rBV2	37266	43760	1.89%	0.347%
43	13.968	2016	2020	2028	rBV	387418	388460	16.73%	3.083%
44	15.445	2266	2271	2279	rBV	262797	338178	14.57%	2.684%

Sum of corrected areas: 12599745

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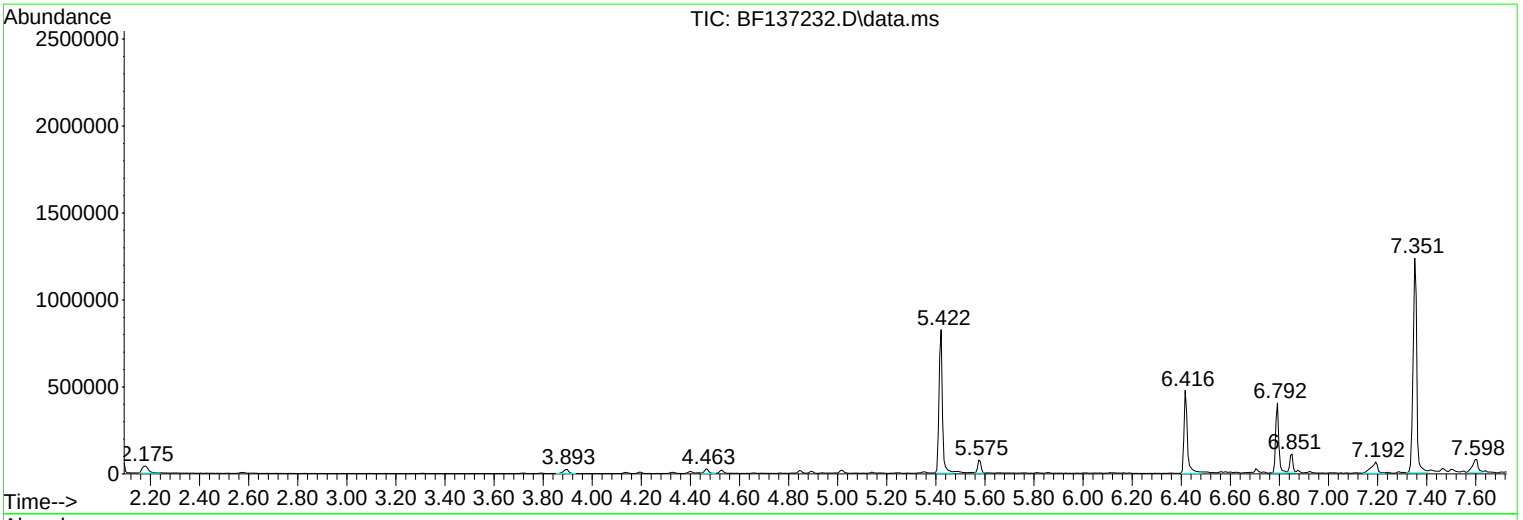
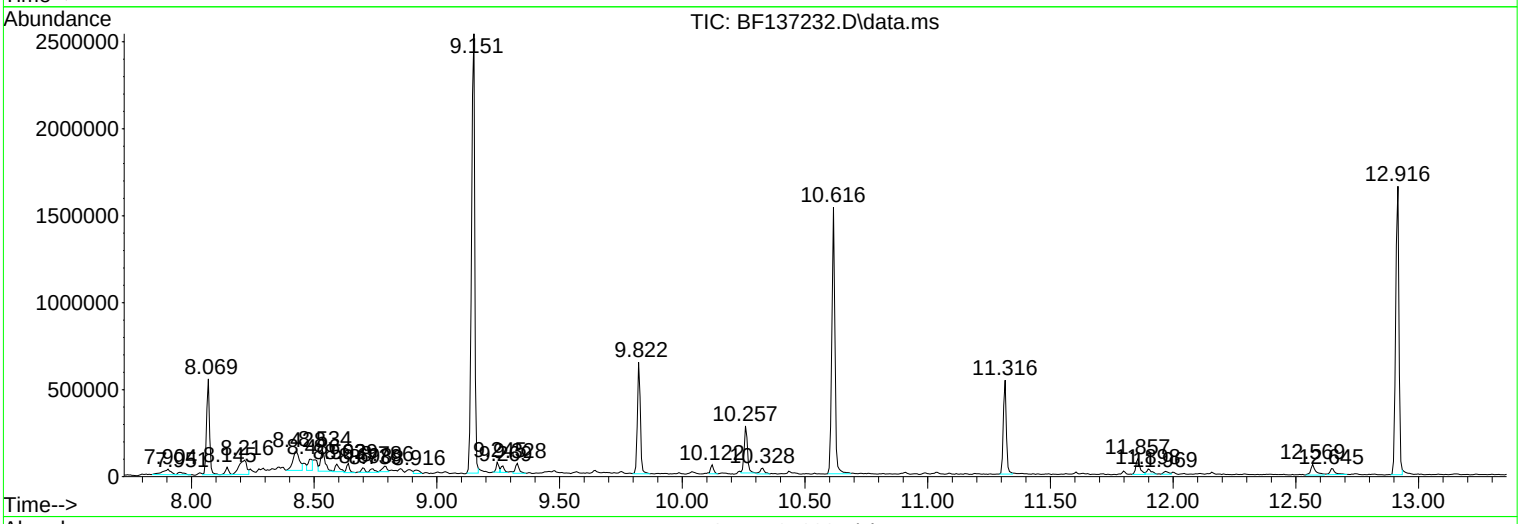
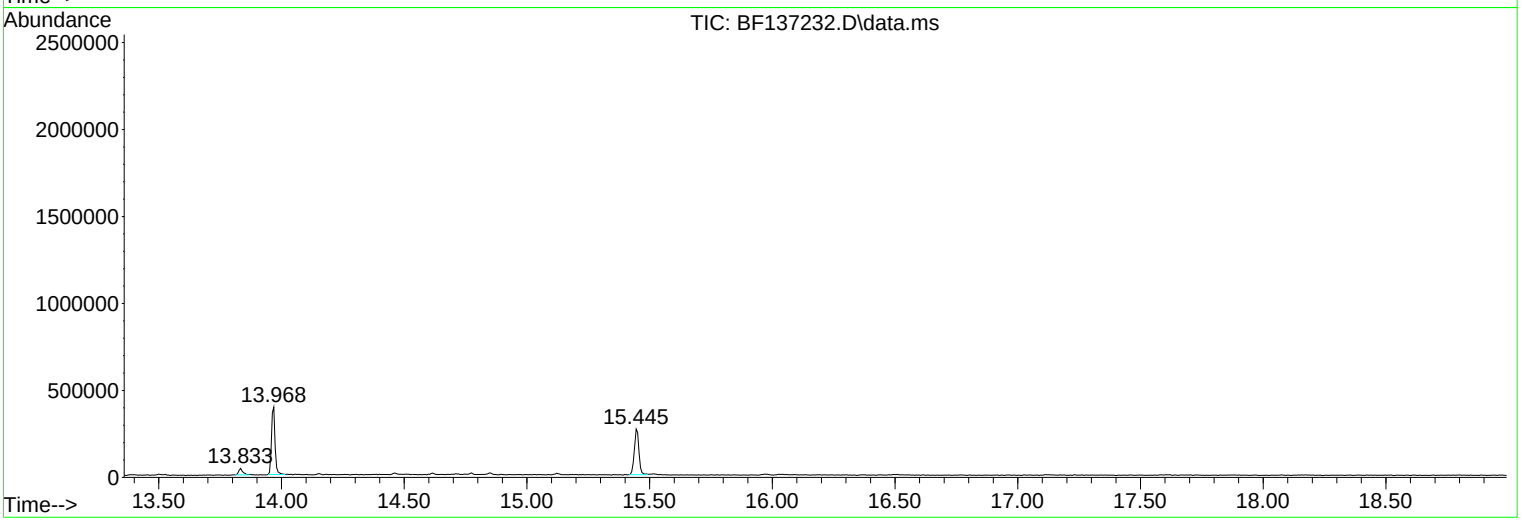
Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020124\
Data File : BF137232.D
Acq On : 01 Feb 2024 15:22
Operator : CG\JU
Sample : P1294-01
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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

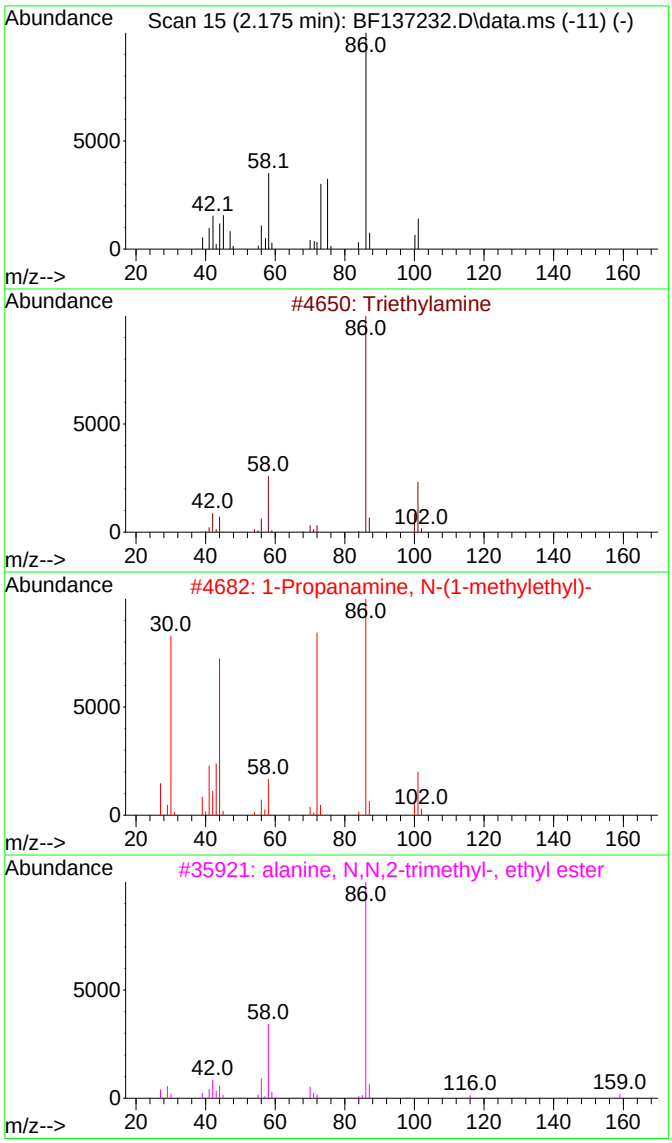
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

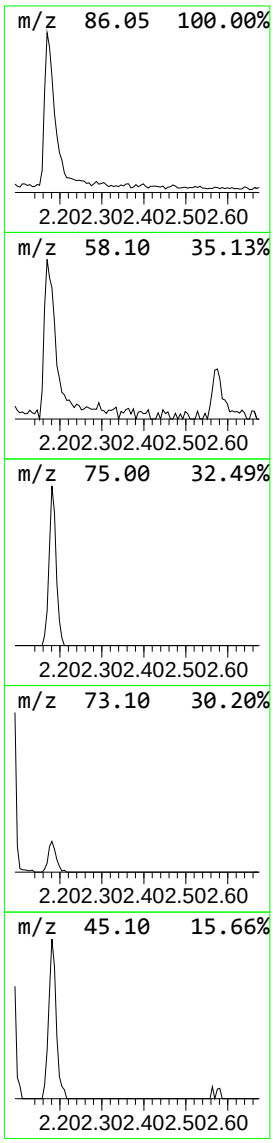
****

Peak Number 1 Triethylamine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	4.08 ng	72340	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethylamine	101	C6H15N	000121-44-8	62
2	1-Propanamine, N-(1-methylethyl)-	101	C6H15N	021968-17-2	53
3	alanine, N,N,2-trimethyl-, ethyl...	159	C8H17NO2	1000404-38-4	50
4	Tetraethylammonium chloride	165	C8H20ClN	000056-34-8	50
5	D-Alloisoleucine	131	C6H13NO2	001509-35-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020124\
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Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

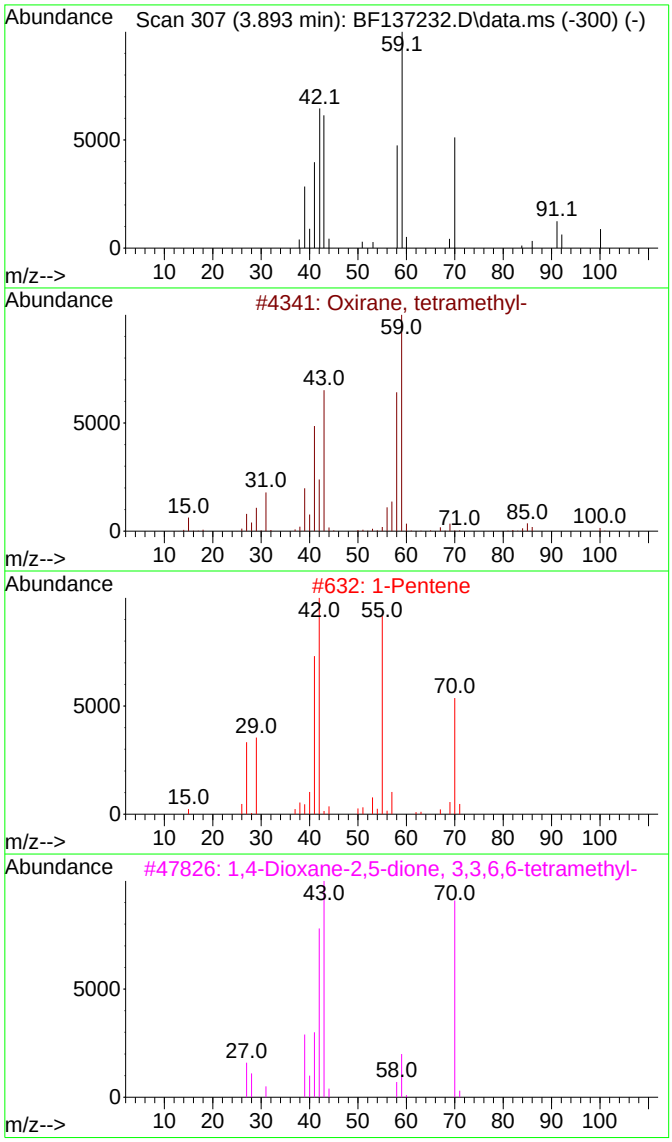
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

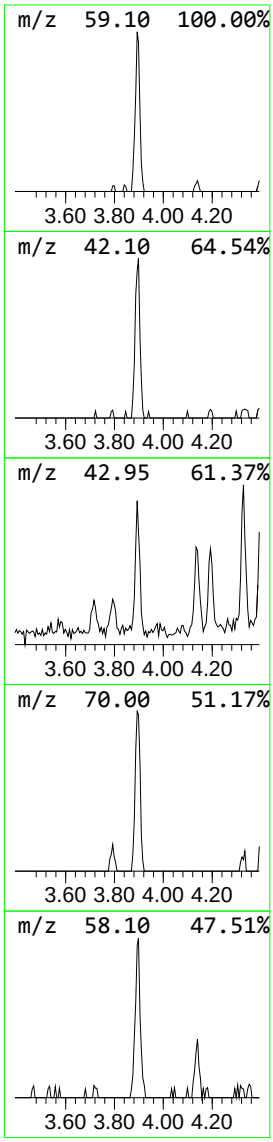
****

Peak Number 2 unknown3.893 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.893	2.09 ng	37162	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	47
2	1-Pentene	70	C5H10	000109-67-1	22
3	1,4-Dioxane-2,5-dione, 3,3,6,6-t...	172	C8H12O4	006713-72-0	12
4	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	10
5	Oxirane, 2-methyl-2-(1-methyleth...	100	C6H12O	072221-03-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020124\
Data File : BF137232.D
Acq On : 01 Feb 2024 15:22
Operator : CG\JU
Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

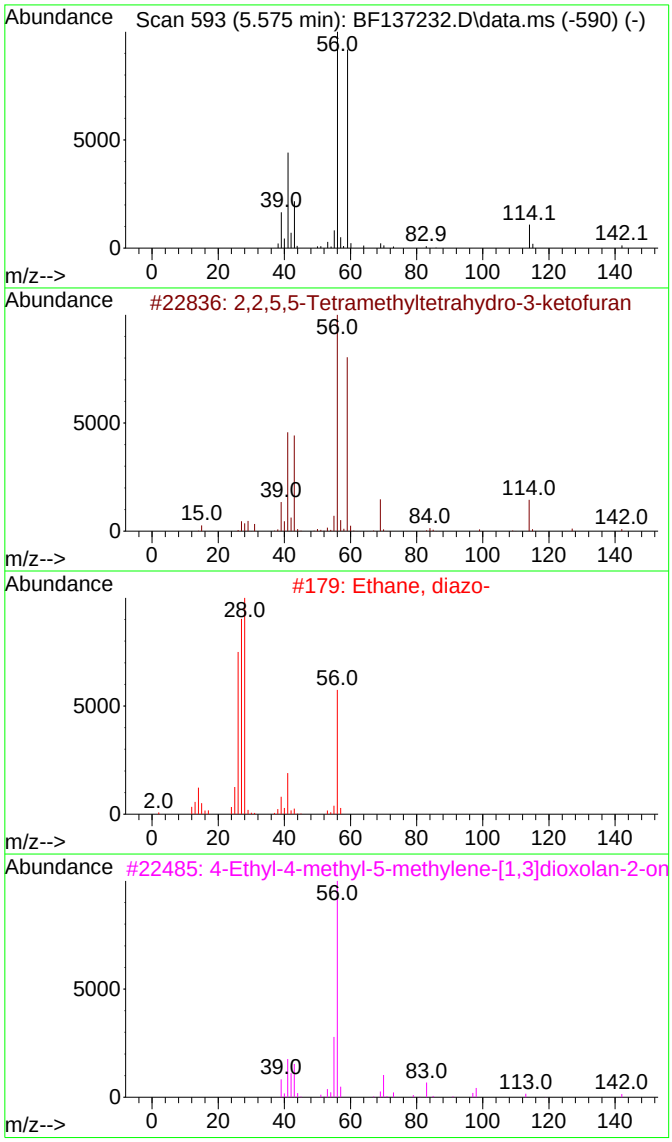
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

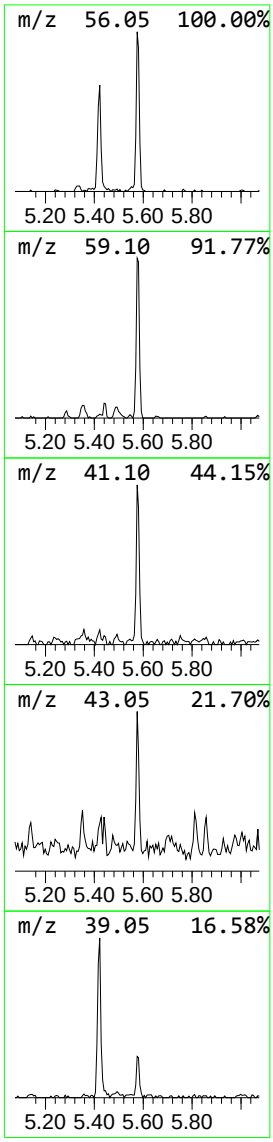
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,2,5,5-Tetramethyltetrahyd... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.575	3.96 ng	70303	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,5,5-Tetramethyltetrahydro-3-...	142	C8H14O2	005455-94-7	72
2	Ethane, diazo-	56	C2H4N2	001117-96-0	32
3	4-Ethyl-4-methyl-5-methylene-[1,...	142	C7H10O3	080956-52-1	9
4	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
5	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	9





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Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

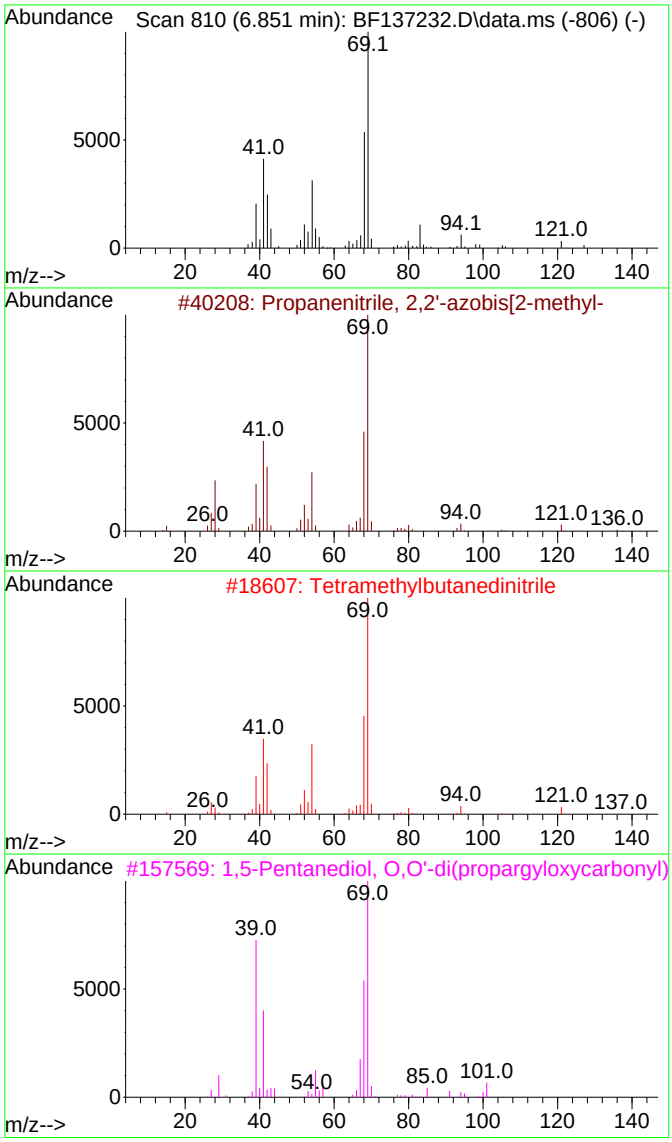
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

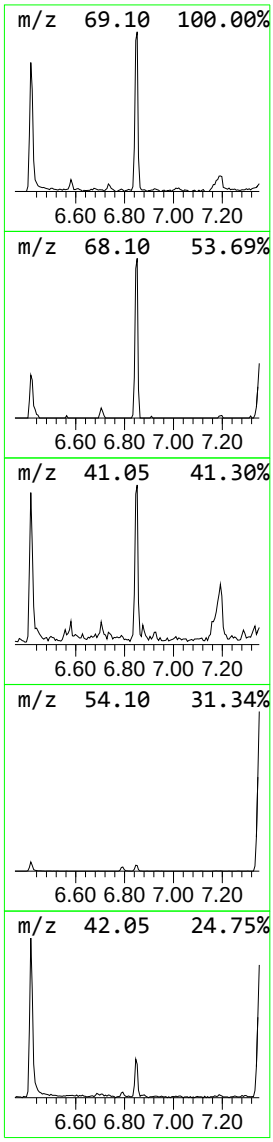
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanenitrile, 2,2'-azobis... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.851	5.02 ng	89134	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanenitrile, 2,2'-azobis[2-me...	164	C8H12N4	000078-67-1	86
2	Tetramethylbutanedinitrile	136	C8H12N2	003333-52-6	86
3	1,5-Pentanediol, O,O'-di(proparg...	268	C13H16O6	1000331-35-4	40
4	Acetic acid, trifluoro-, 1,5-pen...	296	C9H10F6O4	000453-44-1	33
5	Isoxazole	69	C3H3NO	000288-14-2	33





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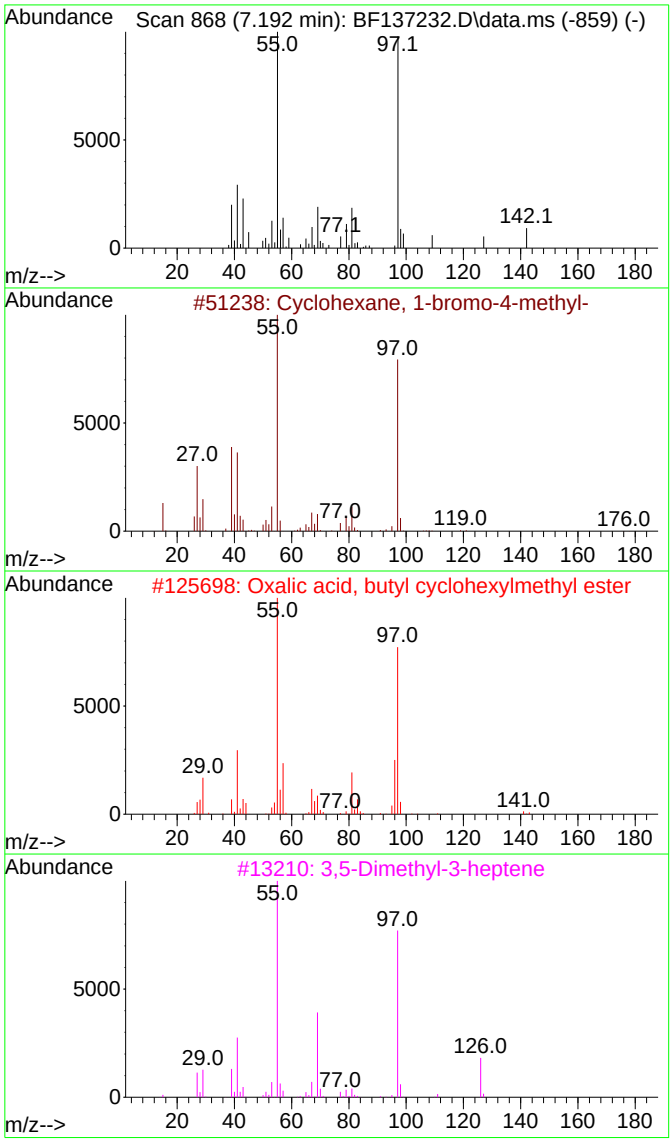
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

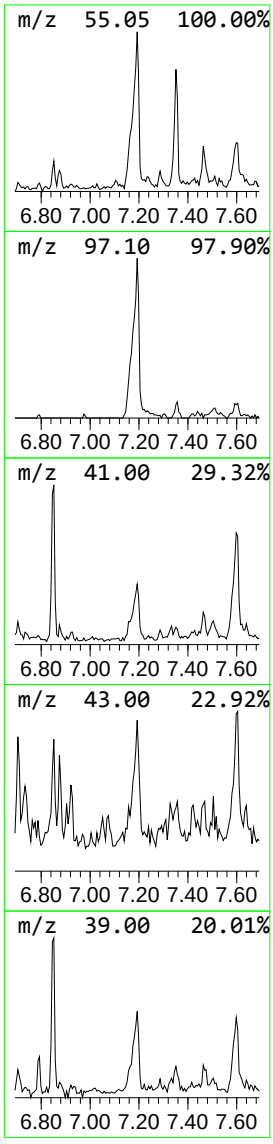
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexane, 1-bromo-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.192	6.71 ng	119000	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	72
2	Oxalic acid, butyl cyclohexylmet...	242	C13H22O4	1000309-68-2	64
3	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	59
4	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	59
5	Cyclopropane, 3-chloro-1,1,2,2-t...	132	C7H13Cl	014123-41-2	59





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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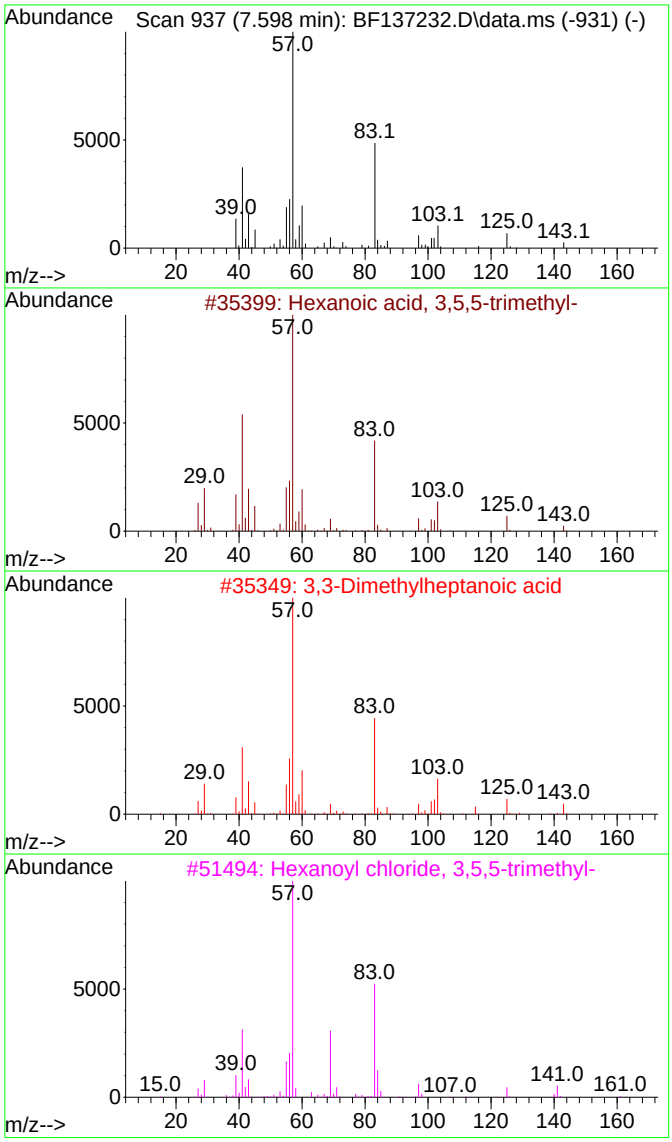
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

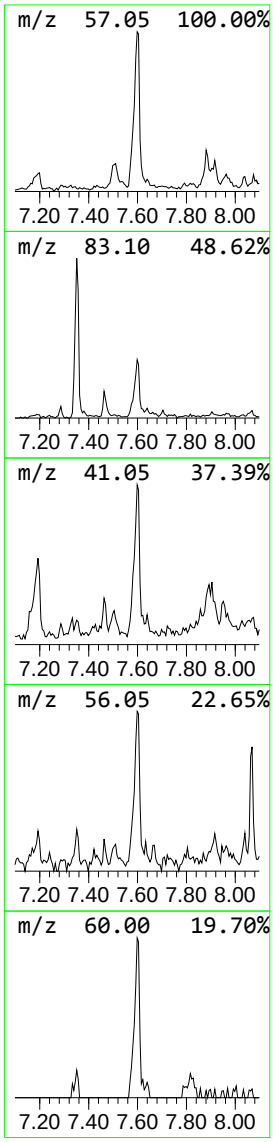
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexanoic acid, 3,5,5-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.598	5.17 ng	119297	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	80
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	72
3	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	50
4	Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	32
5	Hexanal, 3,5,5-trimethyl-	142	C9H18O	005435-64-3	23





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Data File : BF137232.D
Acq On : 01 Feb 2024 15:22
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Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

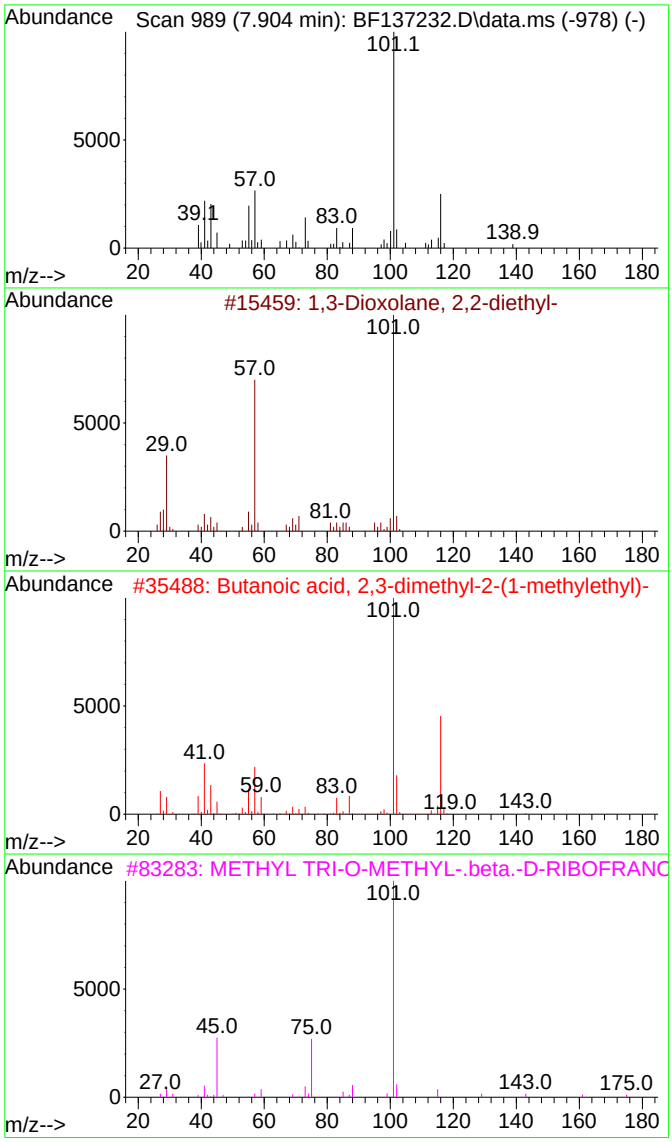
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

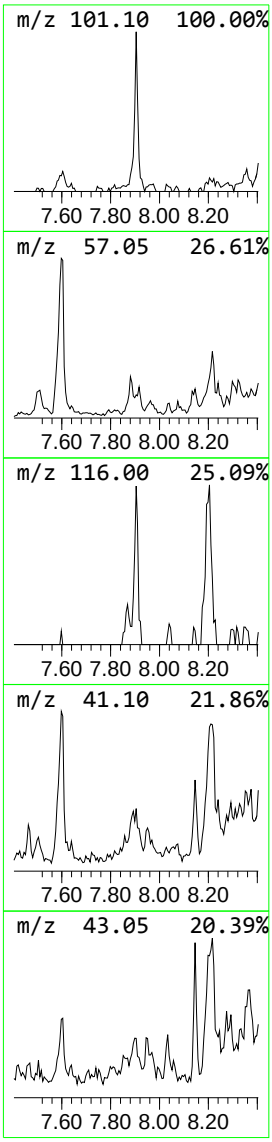
****

Peak Number 7 unknown7.904 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.904	3.21 ng	74090	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2-diethyl-	130	C7H14O2	004362-57-6	47
2	Butanoic acid, 2,3-dimethyl-2-(1...	158	C9H18O2	023119-04-2	40
3	METHYL TRI-O-METHYL-.beta.-D-RIB...	206	C9H18O5	1000432-02-2	40
4	1,3-Dioxepane, 2-pentadecyl-	312	C20H40O2	041563-29-5	38
5	Cyclopentane, 1,2,3,4,5-pentamet...	220	C10H20O5	029887-59-0	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020124\
Data File : BF137232.D
Acq On : 01 Feb 2024 15:22
Operator : CG\JU
Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

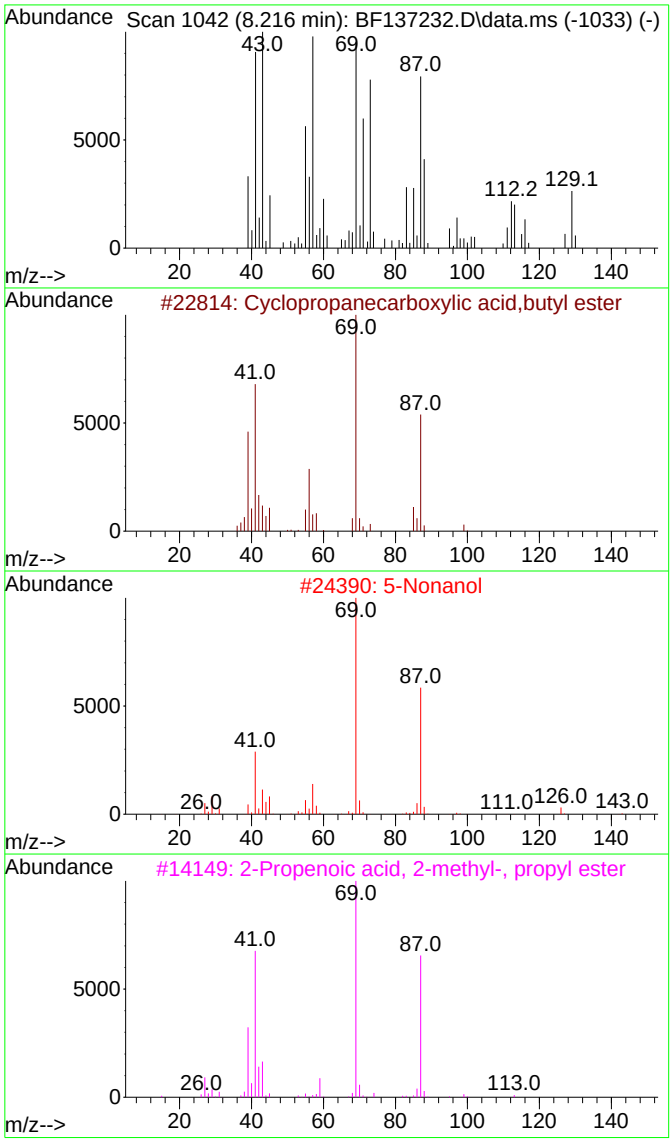
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

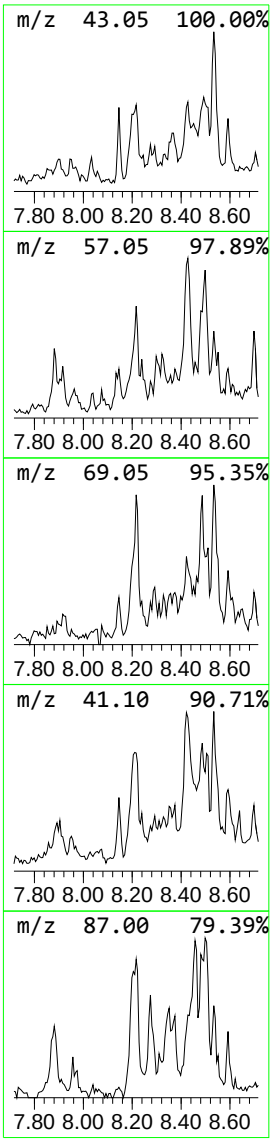
****

Peak Number 8 unknown8.216 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.216	7.72 ng	178102	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid,buty...	142	C8H14O2	054947-39-6	35
2	5-Nonanol	144	C9H20O	000623-93-8	35
3	2-Propenoic acid, 2-methyl-, pro...	128	C7H12O2	002210-28-8	35
4	Ethanone, 1-cyclopentyl-	112	C7H12O	006004-60-0	30
5	2,2-Dimethylpropionic acid, cycl...	170	C10H18O2	1000278-99-9	14





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Data File : BF137232.D
Acq On : 01 Feb 2024 15:22
Operator : CG\JU
Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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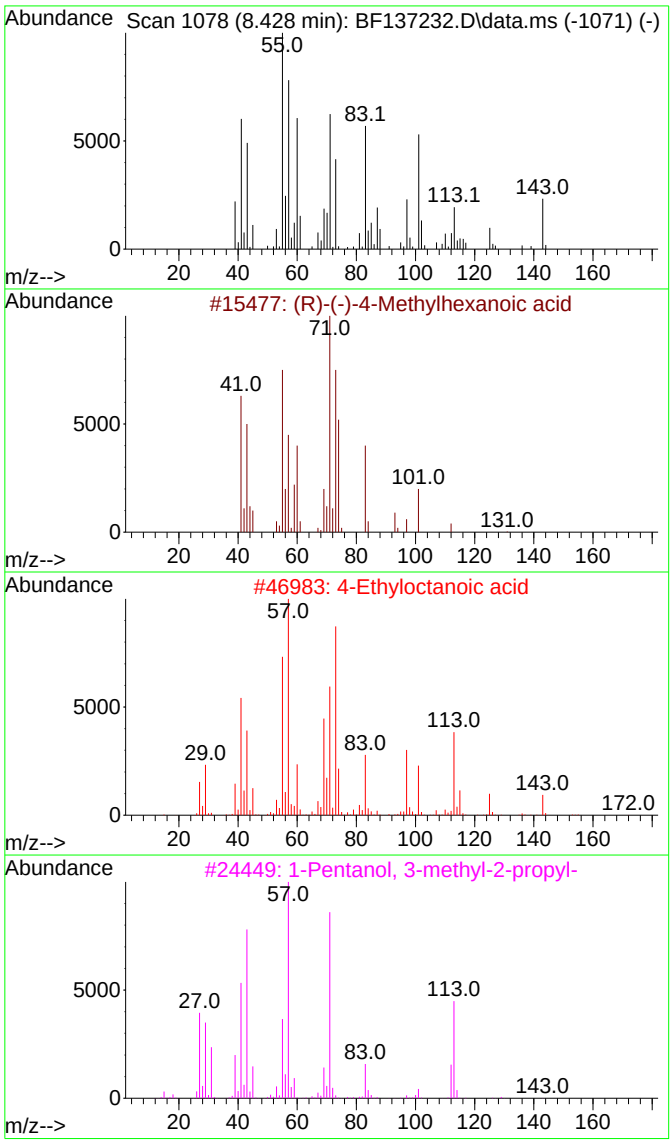
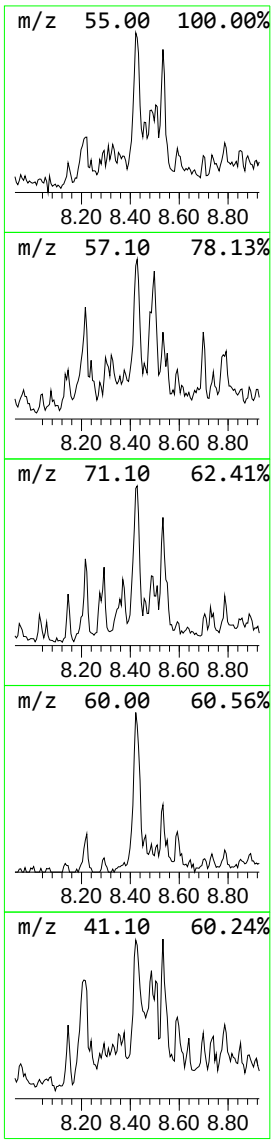
Peak Number 9 unknown8.428 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.428	9.16 ng	211290	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(-)-4-Methylhexanoic acid	130	C7H14O2	052745-93-4	38
2	4-Ethyloctanoic acid	172	C10H20O2	016493-80-4	32
3	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	14
4	2H-1,2-Oxazine,tetrahydro-2-methyl-	101	C5H11NO	022445-43-8	14
5	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	14





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Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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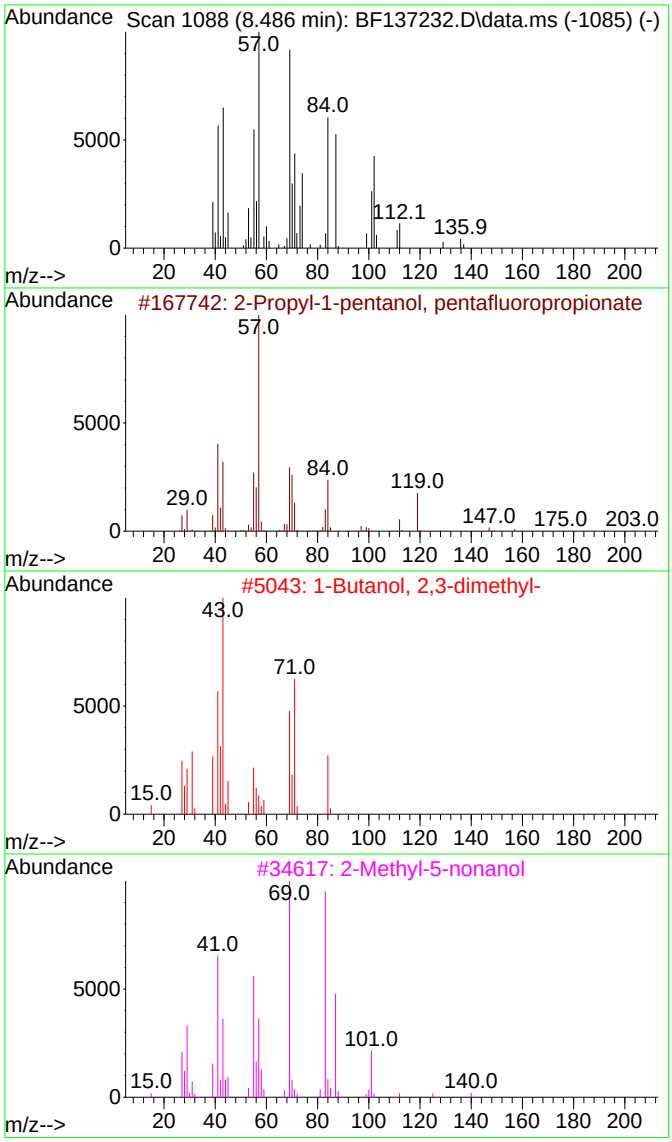
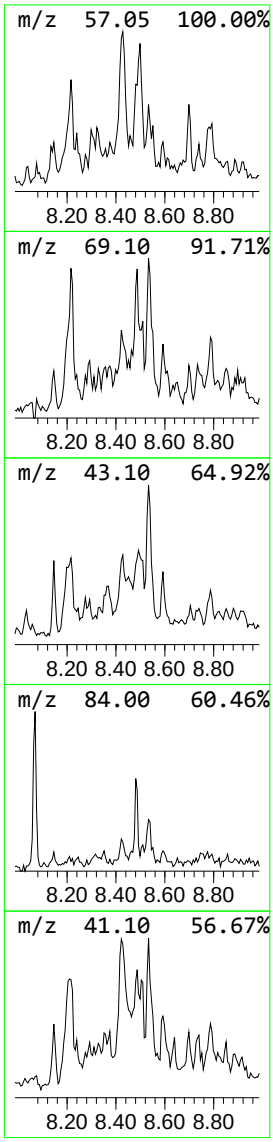
Peak Number 10 unknown8.486 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.486	3.45 ng	79669	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	32
2	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	27
3	2-Methyl-5-nonanol	158	C10H22O	029843-62-7	25
4	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	22
5	2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	22





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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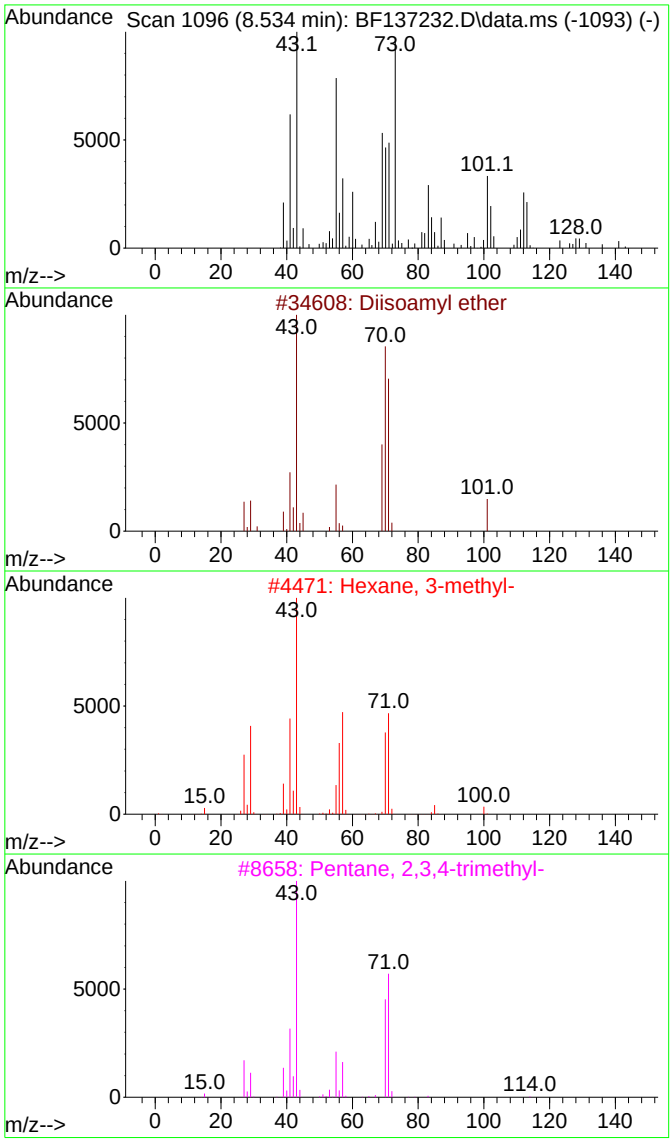
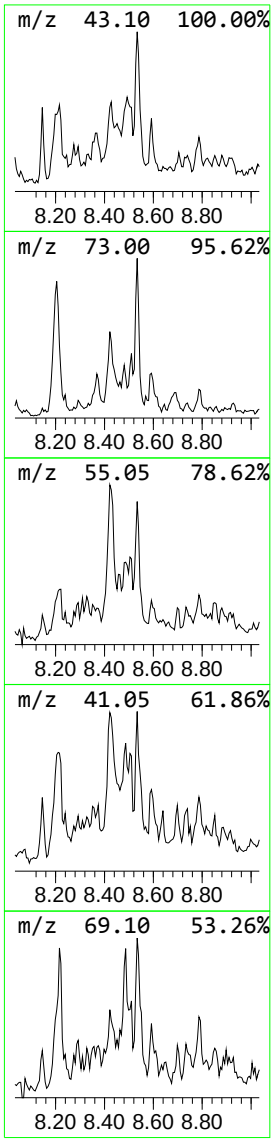
Peak Number 11 unknown8.534 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.534	6.58 ng	151804	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisoamyl ether	158	C10H22O	000544-01-4	27
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	22
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	22
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	22
5	2-Heptene, 4-methyl-, (E)-	112	C8H16	066225-17-0	18





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Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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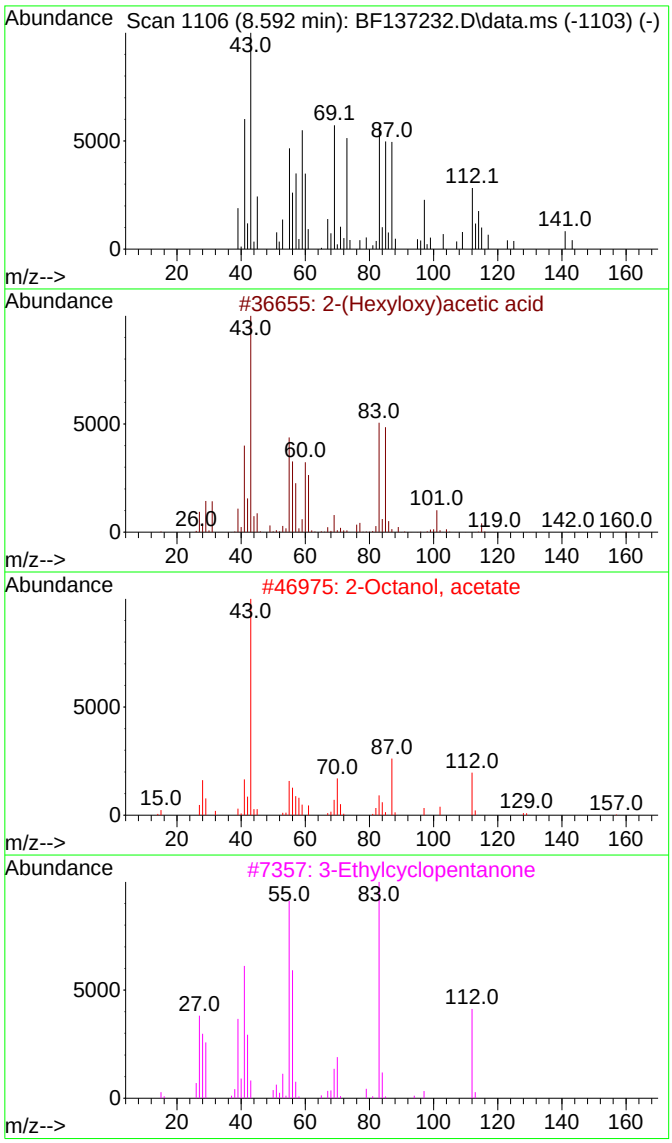
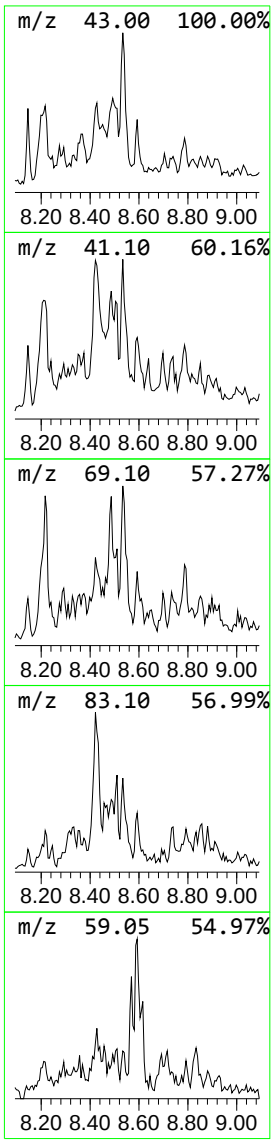
Peak Number 12 unknown8.592 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.592	2.33 ng	53647	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Hexyloxy)acetic acid	160	C8H16O3	057931-25-6	35
2	2-Octanol, acetate	172	C10H20O2	002051-50-5	22
3	3-Ethylcyclopentanone	112	C7H12O	010264-55-8	14
4	3-Methyl-3-hexen-2-ol	114	C7H14O	076966-27-3	11
5	Acetic acid, ethoxy-	104	C4H8O3	000627-03-2	10





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Operator : CG\JU
Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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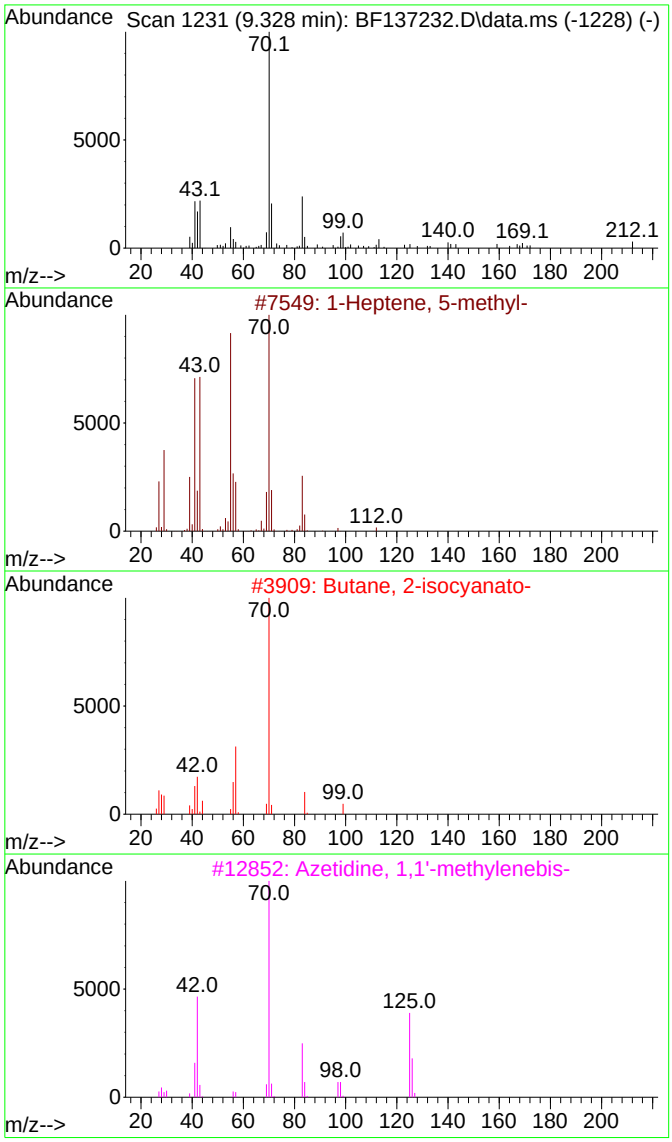
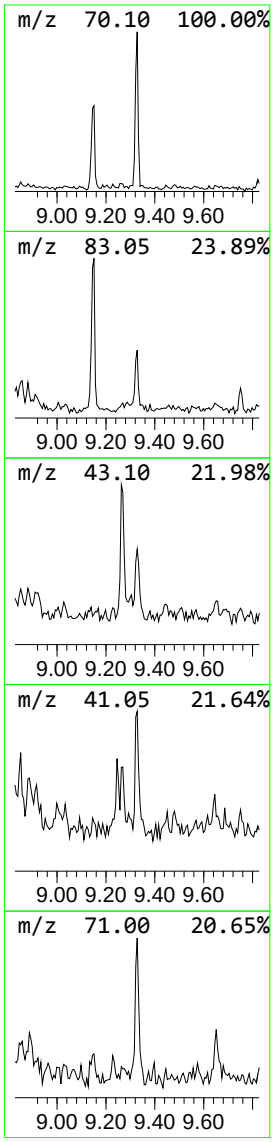
Peak Number 13 1-Heptene, 5-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.328	2.22 ng	59786	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptene, 5-methyl-	112	C8H16	013151-04-7	64
2	Butane, 2-isocyanato-	99	C5H9NO	015585-98-5	50
3	Azetidine, 1,1'-methylenebis-	126	C7H14N2	038455-24-2	50
4	2-Undecene, 3-methyl-, (Z)-	168	C12H24	057024-90-5	40
5	2-Undecene, 3-methyl-, (E)-	168	C12H24	074630-47-0	39





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Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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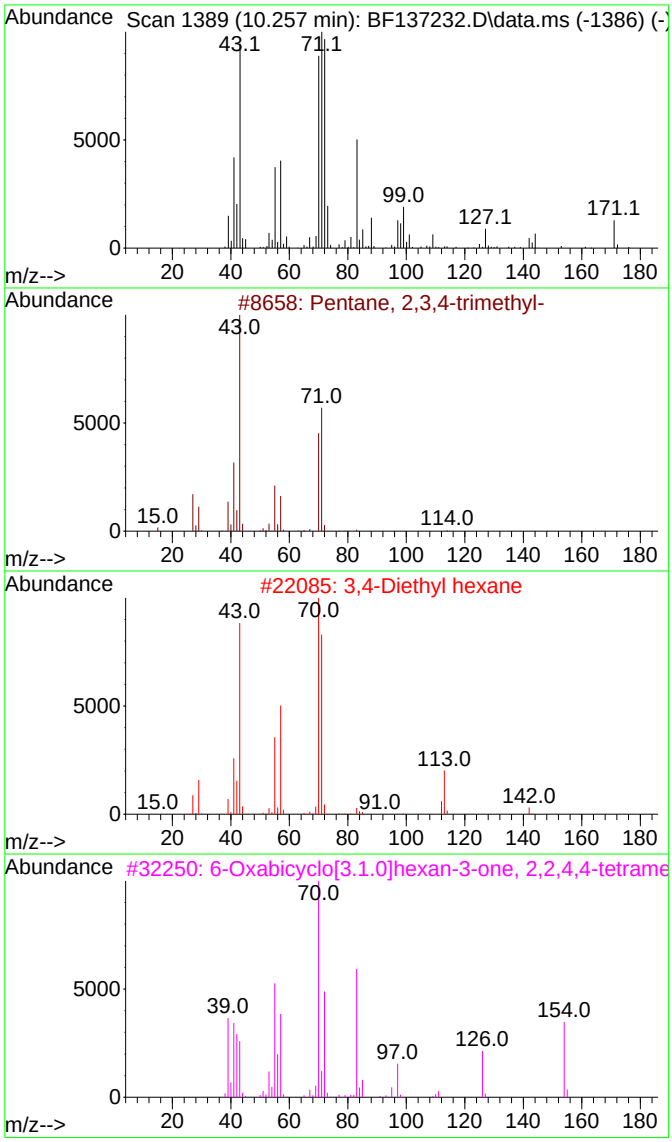
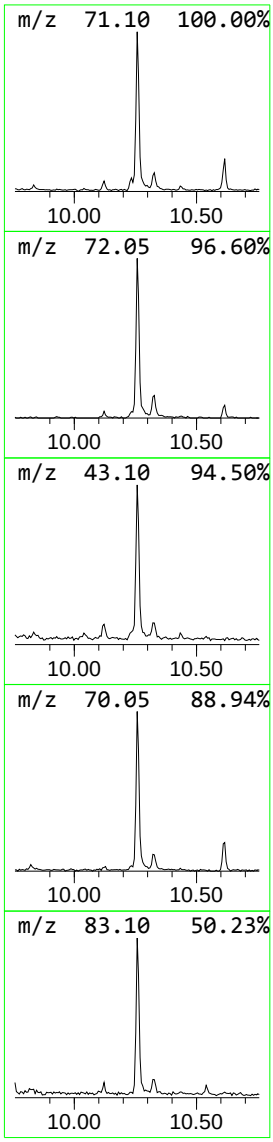
Peak Number 14 unknown10.257 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.257	9.17 ng	247471	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38
2	3,4-Diethyl hexane	142	C10H22	019398-77-7	38
3	6-Oxabicyclo[3.1.0]hexan-3-one, ...	154	C9H14O2	097455-13-5	38
4	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	35
5	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	35





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Acq On : 01 Feb 2024 15:22
Operator : CG\JU
Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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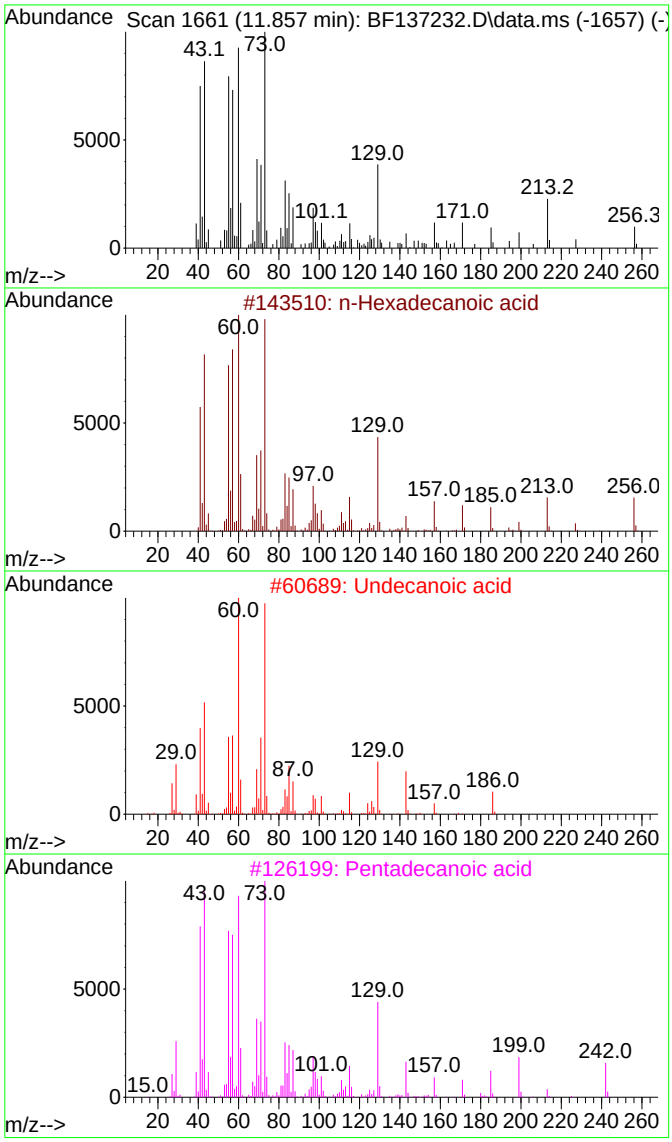
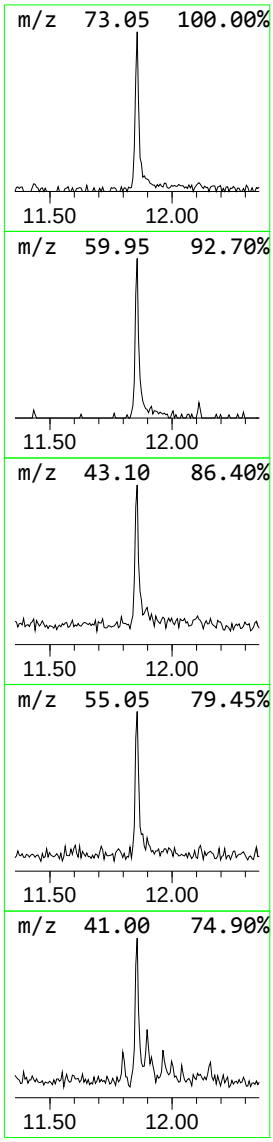
Peak Number 15 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	4.68 ng	108296	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Undecanoic acid	186	C11H22O2	000112-37-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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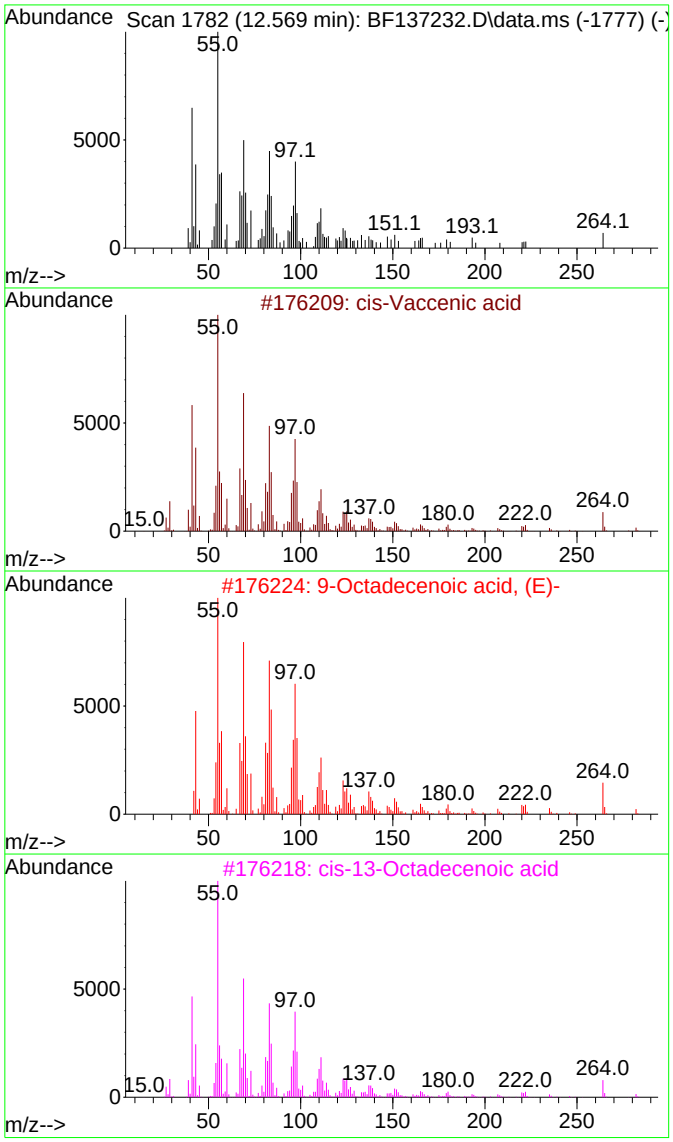
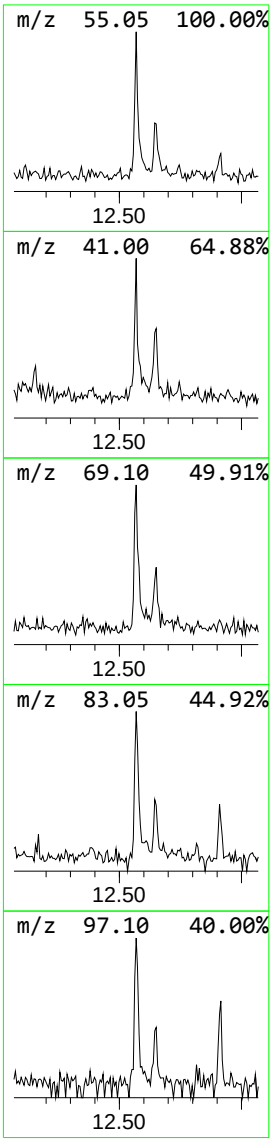
Peak Number 16 cis-Vaccenic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	3.74 ng	86499	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	87
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	87
4	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	87
5	Palmitoleic acid	254	C16H30O2	000373-49-9	80





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Acq On : 01 Feb 2024 15:22
Operator : CG\JU
Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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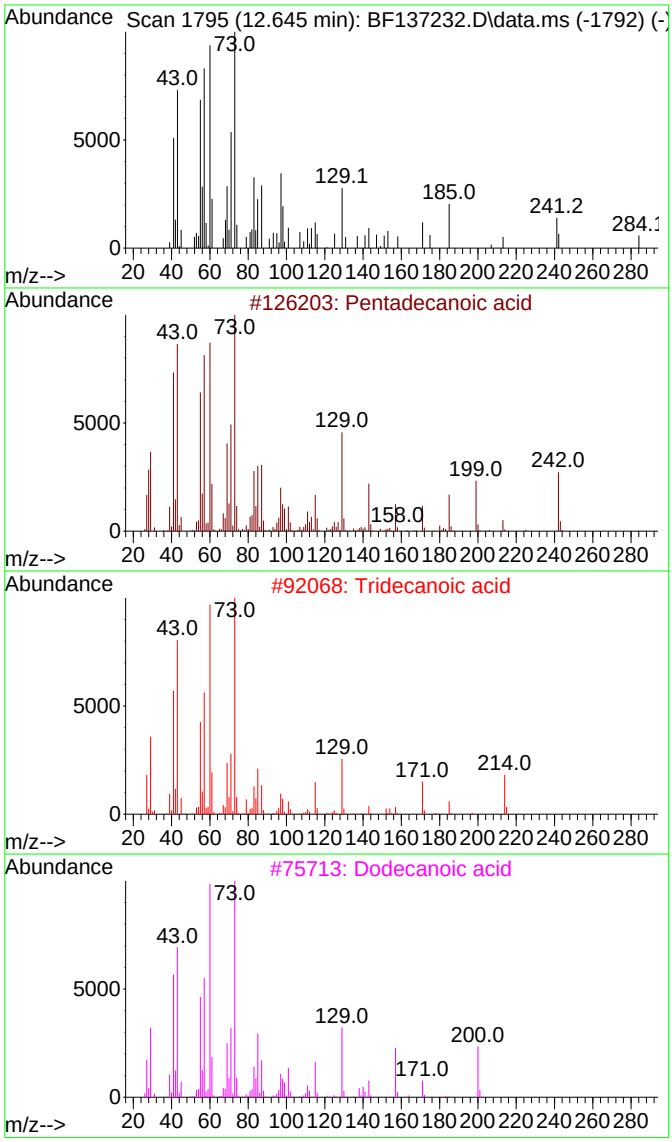
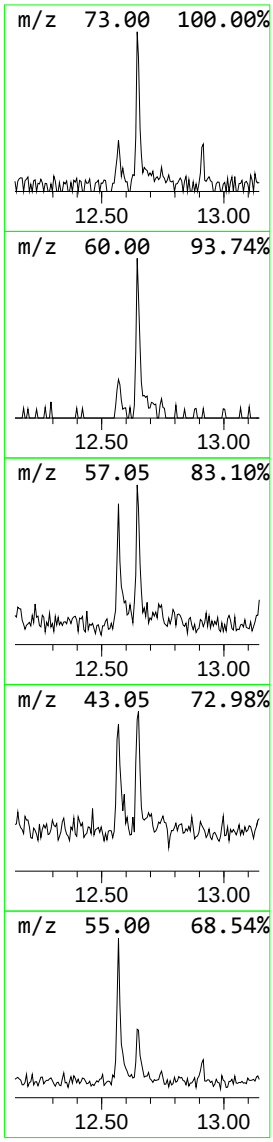
Peak Number 17 Pentadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.49 ng	48374	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	53
3	Dodecanoic acid	200	C12H24O2	000143-07-7	50
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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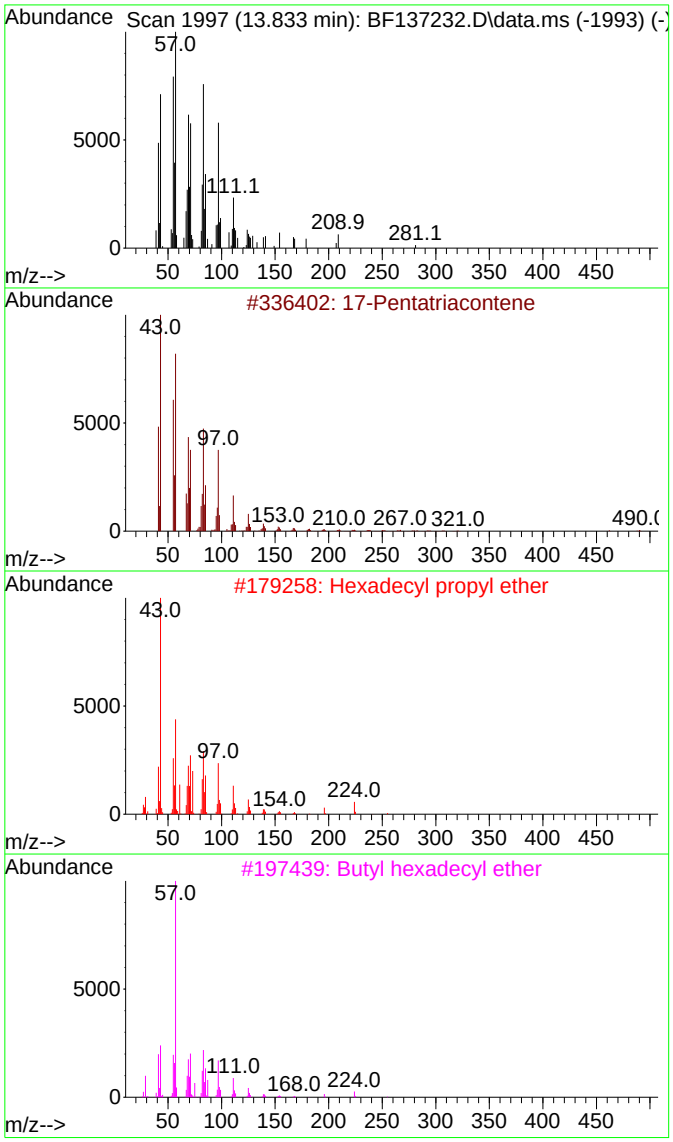
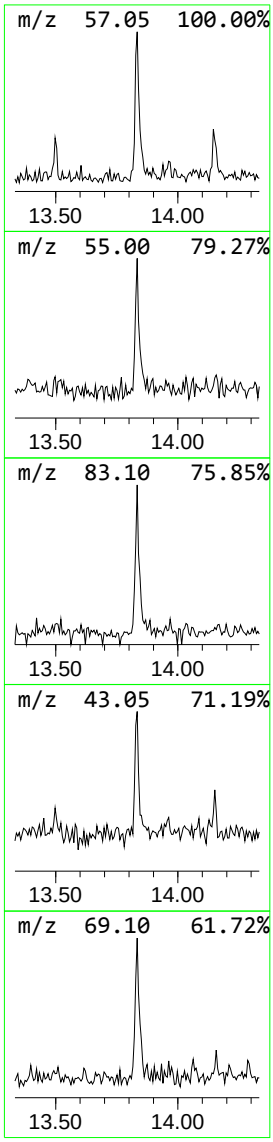
Peak Number 18 17-Pentatriacontene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	2.25 ng	43760	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	90
2	Hexadecyl propyl ether	284	C19H40O	1000406-27-9	87
3	Butyl hexadecyl ether	298	C20H42O	1010406-40-5	87
4	1-Octadecanol	270	C18H38O	000112-92-5	83
5	Behenic alcohol	326	C22H46O	000661-19-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020124\
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Acq On : 01 Feb 2024 15:22
Operator : CG\JU
Sample : P1294-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MMW-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Triethylamine	2.175	4.1	ng	72340	1	6.792	354770	20.0
unknown3.893	3.893	2.1	ng	37162	1	6.792	354770	20.0
2,2,5,5-Tetrame...	5.575	4.0	ng	70303	1	6.792	354770	20.0
Propanenitrile,...	6.851	5.0	ng	89134	1	6.792	354770	20.0
Cyclohexane, 1-...	7.192	6.7	ng	119000	1	6.792	354770	20.0
Hexanoic acid, ...	7.598	5.2	ng	119297	2	8.069	461388	20.0
unknown7.904	7.904	3.2	ng	74090	2	8.069	461388	20.0
unknown8.216	8.216	7.7	ng	178102	2	8.069	461388	20.0
unknown8.428	8.428	9.2	ng	211290	2	8.069	461388	20.0
unknown8.486	8.486	3.5	ng	79669	2	8.069	461388	20.0
unknown8.534	8.534	6.6	ng	151804	2	8.069	461388	20.0
unknown8.592	8.592	2.3	ng	53647	2	8.069	461388	20.0
1-Heptene, 5-me...	9.328	2.2	ng	59786	3	9.822	539506	20.0
unknown10.257	10.257	9.2	ng	247471	3	9.822	539506	20.0
n-Hexadecanoic ...	11.857	4.7	ng	108296	4	11.316	462697	20.0
cis-Vaccenic acid	12.569	3.7	ng	86499	4	11.316	462697	20.0
Pentadecanoic acid	12.645	2.5	ng	48374	5	13.969	388460	20.0
17-Pentatriacon...	13.833	2.3	ng	43760	5	13.969	388460	20.0